

**Department of Electrical and Computer Engineering**

**Center for Integrated Bio and Nano Systems**

**Friday, October 6, 2017**

**11:15 a.m. (Refreshments served at 12:15 pm)**

**Room: CBB 104**

## **Analysis and design of materials for advanced batteries**

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**Abstract:** Energy storage devices are important not only for further developments and for practical uses of renewable energies but also for many other applications in medicine, electronics, electrical vehicles, and the electrical grid. Electrochemical cells involve electrode/electrolyte interfaces where fundamental physical chemistry and reactions problems take place. Understanding such interfaces is crucial for controlling them. In this talk, I will refer to our research on understanding interfacial phenomena for lithium-ion and lithium-sulfur batteries. Our work uses first-principles computational methods such as density functional theory and ab initio molecular dynamics simulations to characterize such interfaces and elucidate reaction mechanisms. I will discuss the integration of our work with collaborative work done using modern characterization surface science in situ techniques.

**Bio:** Perla B. Balbuena is Professor of Chemical Engineering at Texas A&M University since 2004 and has joint appointments in the Department of Materials Science and Engineering and in the Department of Chemistry. Previously she was Assistant and then Associate Professor at the Department of Chemical Engineering at the University of South Carolina. Her research focuses on the first principles analysis and characterization of materials for catalysis, separations, and energy storage and conversion. She has published more than 250 scientific papers in her field of research. Dr. Balbuena's research is currently funded by the US Department of Energy Vehicle Technologies Office (Battery Materials Research), by the Catalysis Division of Basic Energy Sciences, and by Qatar Environment & Energy Research Institute.

Contact Prof. Yan Yao ([yyao4@central.uh.edu](mailto:yyao4@central.uh.edu)) if you would like to arrange for a time to meet with Dr. Balbuena.